SUPPORTING INFORMATION

The crystal structure of the "pentamethylcyclopentadienyl cation" is that of the pentamethylcyclopentyl cation

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Summary of Theoretical Results

All calculations done with the Gaussian 98[i] package of programs. Each molecule/ion was fully optimized in the indicated symmetry. Bond lengths are listed in Å and angles are in degrees.

B3PW91[ii]/6-311G(d)

	Symmetry	Ring Protons	Energy (au)	Relative Energy (kcal/mol)
$[C_5Me_5H_2]^+$	C_1	trans-alpha	-390.991443	0
$[C_5Me_5H_2]^+$	C_1	cis-alpha	-390.989241 6	1.38
$[C_5Me_5H_2]^+$	C_1	trans-beta	-390.948601 7	26.88
$[C_5Me_5H_2]^+$	C_1 (approx C_s)	cis-beta	-390.948634 4	26.86

[i] GAUSSIAN 98 (Revision A.11.1) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, P. Salvador, J. J. Dannenberg, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2001.

[ii] (a) A. D. Becke, *J. Chem. Phys.*, **1993**, *98*, 5648. (b) A. D. Becke, *Phys. Rev. A*, **1988**, *38*, 3098. (c) J. P. Perdew and Y. Wang, *Phys. Rev. B*, **1992**, *45*, 13244.